1 Making a new lattice

Given a set of cartesian basis vectors $\mathbf{L}$ and a matrix $\mathbf{M}$ in Hermite normal form, construct a new lattice

$$\mathbf{L}' = \mathbf{LM} \tag{1}$$

The integer matrix $\mathbf{M}$ has the following form:

$$\mathbf{M} = \begin{pmatrix} a & d & e \\ 0 & b & f \\ 0 & 0 & c \end{pmatrix} \tag{2}$$

with

$$\begin{aligned}
d, e &\in \left[-(a-1)/2, -(a-1)/2+1, \cdots, (a-1)/2\right] ; a \text{ odd} && (3)\\
d, e &\in \left[-a/2+1, -a/2+2, \cdots, a/2\right], a \text{ even} && (4)\\
f &\in \left[-(b-1)/2, -(b-1)/2+1, \cdots, (b-1)/2\right] ; b \text{ odd} && (5)\\
f &\in \left[-a/2+1, -a/2+2, \cdots, a/2\right] ; b \text{ even} && (6)\\
a &> 0 && (7)\\
b &> 0 && (8)\\
c &> 0 && (9)\\
& && (10)
\end{aligned}$$

The determinant of $\mathbf{M}$ describes the volume ratio of the newly chosen cell to the originalk cell. As the determinant of $\mathbf{M}$ is equal to abc, all matrices with a certain determinant Δ can be easely constructed by finding all triples (a, b, c) for which $\Delta = abc$. A simple use of a brute force integer factorisation (known as trial factorisation) algorithm, can return these triples fast.

The construction of a new lattice is thus relatively straightforward.

2 Unit cell comparison

Say we have a basis $\mathbf{L}_r$ in the reference setting. Transform it to the Niggli setting:

$$\mathbf{L}_n = \mathbf{R}_n \mathbf{L}_r \mathbf{R}_n^{-1} \tag{11}$$

Do the same for a *target* lattice:

$$\mathcal{L}_n = \mathcal{R}_n \mathcal{L}_r \mathcal{R}_n^{-1} \tag{12}$$

We are looking for a matrix $\mathbf{M}$ and affine (*similarity*) transform of the lattice $\mathbf{S}$ for which

$$\mathcal{L}_n \approx \mathbf{S}\mathbf{L}_n\mathbf{M}\mathbf{S}^{-1} \tag{13}$$

If one desires to explore all matrices $\mathbf{M}$ with determinant equal to 10, only 217 matrices need to be checked. The big computational cost are the number of affine transformations to check. One hopes all unimodular matrices are sufficient.

3 Basic transformations

Here I quickly derive/review some basic transformations commonly used in crystallography. The main assumption is that the transformation does not involve a translational component.

3.1 The direct space

The matrix $\mathbf{L}$ with column vectors describes the lattice. L is also known as the orthogonalization matrix:

$$\mathbf{r} = \mathbf{L}\mathbf{x} \tag{14}$$

$\mathbf{r}$ is a (column) vector with cartesian coordinates. $\mathbf{x}$ is a colmun vector with so called fractional coordinates.

The metrical matrix $\mathbf{G}$ is defined as

$$\mathbf{G} = \mathbf{L}^T\mathbf{L} \tag{15}$$

and is commenly introduced by showing how to computre dot product of real space quanitities.

$$\begin{aligned} \mathbf{r}_1^T\mathbf{r}_2 &= (\mathbf{A}\mathbf{x}_1)^T\mathbf{A}\mathbf{x}_2 && (16)\\ &= \mathbf{x}_1^T\mathbf{A}^T\mathbf{A}\mathbf{x}_2 && (17)\\ &= \mathbf{x}_1^T\mathbf{G}\mathbf{x}_2 && (18) \end{aligned}$$

If a new lattice is defined by actrion of matrix $\mathbf{M}$, investigate how other quantities change. Repeat the basic expression involving the hermite normal form matrix (but can be any other transform actually)

$$\mathbf{L}' = \mathbf{L}\mathbf{M} \tag{19}$$

The metrical matrix changes as follows:

$$
\begin{aligned}
\mathbf{G}' &= (\mathbf{L}')^T\mathbf{L}' && (20)\\
&= (\mathbf{LM})^T\mathbf{LM} && (21)\\
&= \mathbf{M}^T\mathbf{L}^T\mathbf{LM} && (22)\\
&= \mathbf{M}^T\mathbf{GM} && (23)
\end{aligned}
$$

If we fix a cartesian coordinate and change basis, we find out the transformation law for the fractional coordinates after choosing a new set of basis vectors:

$$
\begin{aligned}
\mathbf{r} &= \mathbf{Lx} && (24)\\
&= \mathbf{L}'\mathbf{x}' && (25)\\
\mathbf{Lx} &= \mathbf{L}'\mathbf{x}' && (26)\\
\mathbf{Lx} &= \mathbf{LMx}' && (27)\\
\mathbf{x} &= \mathbf{Mx}' && (28)\\
\mathbf{x}' &= \mathbf{M}^{-1}\mathbf{x} && (29)
\end{aligned}
$$

Deriving transformation laws for symmetry operations, is done as follows

$$
\begin{aligned}
\mathbf{x}_p &= \mathbf{Rx} + \mathbf{t} && (30)\\
\mathbf{Mx}'_p &= \mathbf{RMx}' + \mathbf{t} && (31)\\
\mathbf{x}'_p &= \mathbf{M}^{-1}\mathbf{RMx}' + \mathbf{M}^{-1}\mathbf{t} && (32)
\end{aligned}
$$

Which obviously leads to

$$
\begin{aligned}
\mathbf{R}' &= \mathbf{M}^{-1}\mathbf{RM} && (33)\\
\mathbf{t}' &= \mathbf{M}^{-1}\mathbf{t} && (34)
\end{aligned}
$$

3.2 Reciprocal space

The reciprocal lattice has the following relation to the direct lattice

$$
\mathbf{L}^{*T}\mathbf{L} = \mathbf{I} \qquad (35)
$$

from which follows:

$$\begin{aligned}
\mathbf{L} &= \left(\mathbf{L}^{*T}\right)^{-1} && (36)\\
\mathbf{L}^T\mathbf{L} &= \mathbf{L}^T\left(\mathbf{L}^{*T}\right)^{-1} && (37)\\
\mathbf{G} &= \mathbf{L}^T\left(\mathbf{L}^{*T}\right)^{-1} && (38)\\
\mathbf{G}\mathbf{L}^{*T} &= \mathbf{L}^T && (39)\\
\mathbf{L}^*\mathbf{G} &= \mathbf{L} && (40)
\end{aligned}$$

In a similar manner, one can show

$$\mathbf{L}^* = \mathbf{L}\mathbf{G}^* \tag{41}$$